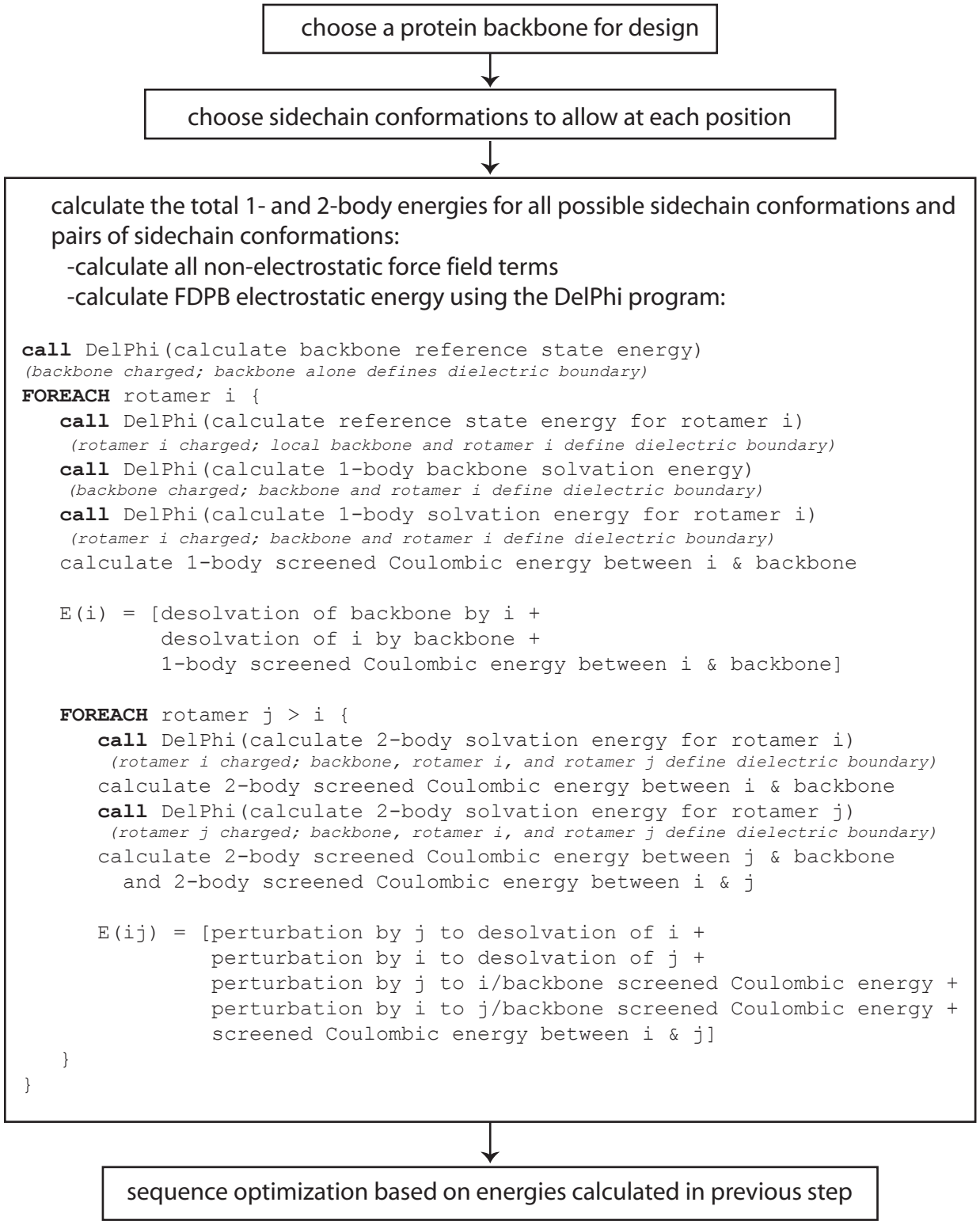

Supplemental Figure 1. Protein design protocol, including one- and two-body FDPB calculations. A simplified version of the protein design procedure shows the step at which electrostatic energies are calculated. Pseudocode for the electrostatics calculation shows the number of times in which the FDPB program DelPhi is called. For screened Coulombic energies, the potential maps from previous calculations are used to obtain screening energies. As described in the methods section, desolvation energies are computed as the difference between folded state and reference state solvation energies. Two-body perturbations for sidechain desolvation and sidechain/backbone screened Coulombic energies are computed as the difference between the respective two-body and one-body energies.